

Studying the Behavior of Crystal Deformation

MOST of the seemingly static and unchanging metals we encounter in our daily lives are anything but unchanging. At the atomic level, metals are a highly complex and ordered arrangement of atoms that have the potential to rearrange themselves, especially when put under extreme strain and stress. Livermore researchers are working to gain a better understanding of how several metals achieve permanent, or plastic, deformation.

Most of the time, atoms self-organize into crystalline lattice structures. A single crystal is composed of millions of these lattices oriented in exactly the same direction. Single crystals are the building blocks of everyday materials, such as the steels used in

automobiles, that are typically polycrystalline; that is, the lattice structures are stacked in many different orientations. Materials scientists at Livermore are using a three-dimensional (3D) image-correlation system and a novel mechanical test system to investigate how metallic single crystals behave under mechanical stress and strain. The researchers, funded by the Laboratory Directed Research and Development Program, are using a new method to look at an old problem. “We are closing in on a body of data that enable some new thinking on crystal plasticity,” says David Lassila, a materials scientist in the Engineering Directorate.

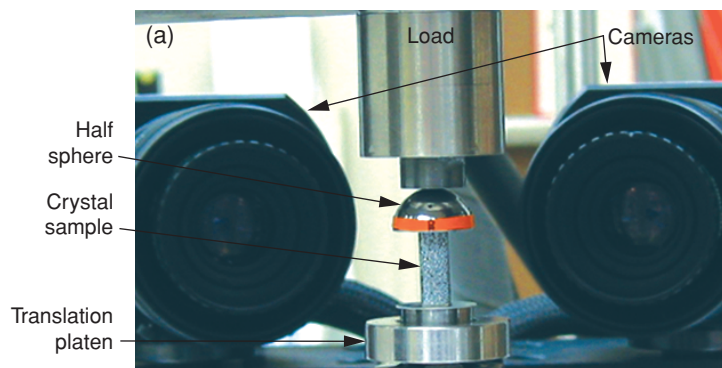
Livermore scientists investigate the structures and properties of various materials to better understand the limits of materials and how their properties may change under certain conditions. This work also enables researchers to design new materials that will have specific desirable properties.

Lassila’s team includes materials scientist Jeff Florando and senior engineering associate Mary LeBlanc, also from Engineering. Their work contributes to Livermore’s mission in support of the National Nuclear Security Administration’s Stockpile Stewardship Program. Key to managing the nation’s aging nuclear weapons stockpile is the development of material-strength models that are accurate under extreme conditions of high pressure, high strain rate, and large extents of strain.

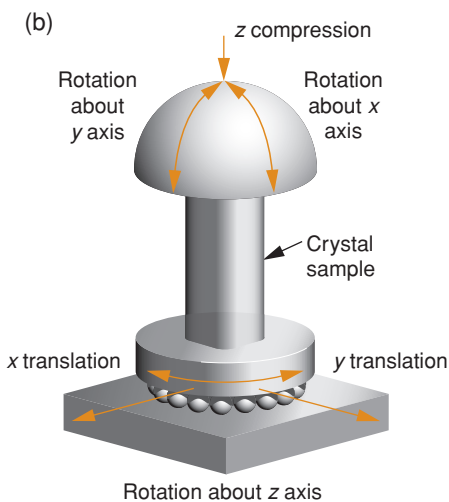
Stepping into the Future

In the past, materials scientists have depended on traditional crystal plasticity theory, which was developed with data from 1D experiments during the 1920s and 1930s. Traditional plasticity theory—Schmid’s Law—is based on the 1D response of thin wires, where only one slip system is active. The dislocation activity is idealized and not representative of real materials, where dislocation activity is much more complex. Lassila’s team is finding traditional theory might lead to experimental results that are not very accurate. “We’re collecting data with the 3D image-correlation system that’s quite different from what we were inferring with traditional theory,” says Florando.

The 3D image-correlation system includes two charge-coupled-device (CCD) cameras that focus on the experimental apparatus. Before the experiment, a single-crystal sample is painted with black dots on a white background, and a half sphere is centered over the sample. When a load is applied to the sample through the half sphere, the six-degrees-of-freedom (6DOF) apparatus allows for tilt



(a) Livermore researchers use three-dimensional image correlation to measure full-field displacements and strains on a crystal sample. Two charge-coupled-device cameras focus on the experimental apparatus and capture images of the material before and after deformation caused by large strains. (b) The experimental apparatus allows the crystal to deform essentially unconstrained in six directions (orange arrows).



in two directions (two degrees), rotation about the compression axis (one degree), and compression in the z direction (one degree). Additionally, the bottom translation platen sits on ball bearings that allow full motion in the x - y plane, adding two more degrees of freedom. As the sample deforms, the two CCD cameras record the positions of the black dots by triangulation.

“We are deforming the lattice through load,” says Florando. “This change is brought about by the atoms moving in a slip plane in response to the stress and strain of the load.” Materials scientists call these atomistic disruptions “dislocations.” In single crystals, slip planes are the preferred planes where dislocations move. The set of slip planes and slip directions in a crystal constitute the slip system. “Materials can slip in many ways,” says Florando. “We’re using the data from the image-correlation system to determine which slip systems are active.” The recorded data are used to create strain maps with various colored bands displaying the inhomogeneities in the crystal deformation.

With the new experimental data, the researchers found that, in general, Schmid’s Law is the exception and not the rule. Interestingly, the plasticity of crystals with different structures to be remarkably similar in their non-Schmid plastic response. The researchers hope to use Livermore’s multiscale-modeling capabilities to understand non-Schmid behavior and establish a more fundamental understanding of the plastic response of metallic single crystals.

Multidirectional Measurements in Real Time

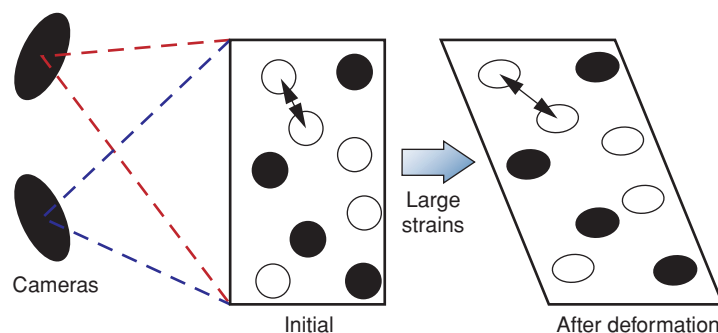
Although other optical techniques for measuring the deformation of materials are available, the team found that image correlation had a number of advantages in the study of single crystals. Image correlation allows researchers to measure larger, full-field strains while tracking the motion of the sample. It also allows them to measure the displacements and displacement gradients in three dimensions.

With a strain gauge, the traditional measuring device, calculations were attainable for only five independent slip systems. Image correlation, however, measures displacements rather than strain. “Using image correlation, we can accurately determine the slip activity for up to eight independent slip systems while the material is deforming,” says Lassila. This additional knowledge leads to a better understanding of how materials fundamentally deform.

If a crystal is oriented such that the slip direction is parallel to a face of the sample, the slip activity for that system can be directly measured. Image-correlation techniques allow for the direct measurement of slip activity by rotating the axes to lie in the direction of the slip plane.

Experimental Insight

The deformation data being collected by the team is essential for direct comparisons and validation of dislocation dynamics simulations. (See *S&TR*, November 2005, pp. 4–11.) Currently, the large-strain deformation behavior of single crystals is not well



In three-dimensional image-correlation experiments, the crystal sample is painted with black dots on a white background. As the sample deforms, the two charge-coupled-device cameras record the relative motion of the black dots, providing local displacement data.

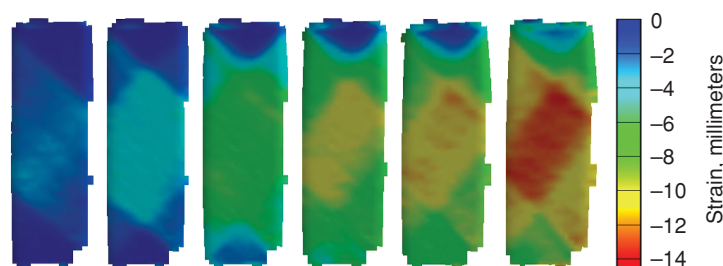


Image-analysis software processes data from three-dimensional image-correlation experiments to create strain maps. Maps from an experiment with a copper sample show axial strains at different stages. The areas represented by the red bands received the highest level of strain.

understood. Because many materials of interest to scientists at Livermore are deformed to relatively large strains, new experimental techniques are needed for measuring the deformation behavior of single crystals under large extents of strain.

“Crystal plasticity models play a key role in multiscale modeling to predict the deformation response of complex materials under various loading conditions,” says Florando. “Insight gained from large-strain experiments has the potential to advance crystal plasticity theory and predictive modeling capabilities.”

—Maurina S. Sherman

Key Words: crystal deformation, dislocation dynamics, metallic single crystals, six degrees of freedom (6DOF), slip systems, strain, stress, three-dimensional (3D) image correlation.

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